

# Reply to Comment on "Violation of Anderson's Theorem for the sign-reversing s-wave state of Iron-Pnictide Superconductors" [arXiv:1012.0414] by Y. Bang

Seiichiro ONARI<sup>1</sup>, and Hiroshi KONTANI<sup>2</sup>

<sup>1</sup> Department of Applied Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.

<sup>2</sup> Department of Physics, Nagoya University and JST, TRIP, Furo-cho, Nagoya 464-8602, Japan.

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We explain that the study of impurity effect in iron pnictides [1] are correctly calculated based on the  $T$ -matrix approximation, contrary to the Comment by Bang[2]. The replacement  $\hat{T}^b$  with  $\hat{T}^b - \hat{I}^b$  proposed by Bang breaks the perturbation theory and is therefore erroneous.

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In Ref.[1], we studied the nonmagnetic impurity effect in the multiorbital model for iron pnictide superconductors. In the sign-reversing  $s$ -wave state ( $s_{\pm}$ ), we found that (i)  $T_c$  is substantially suppressed by the inter-band impurity scattering, since the  $T$ -matrix has large inter-band matrix elements. (ii) This result holds even in the unitary limit, contrary to the fact that (iii) inter-band scattering vanishes in the unitary limit if the bare impurity potential in the band basis  $\hat{I}^b$  is a constant matrix and  $\det\{\hat{I}^b\} \neq 0$  [3]. In iron pnictides, the statement (ii) holds since  $\hat{I}^b$  has large  $\mathbf{k}$ -dependence.

In Ref. [2], Bang complained that the result (iii) is incorrect, that is, he claimed that inter-band scattering exists in the unitary limit even if  $\det\{\hat{I}^b\} \neq 0$ . Here, we explain the formalism of the  $T$ -matrix approximation when  $\hat{I}^b$  is constant, and point out the error in Ref. [2]. The  $T$ -matrix for a single impurity in the band-basis is

$$\hat{T}^b = (\hat{1} - \hat{I}^b \hat{g}_{loc}^b)^{-1} \hat{I}^b, \quad (1)$$

where  $\hat{g}_{loc}$  is the local Green function. In the  $T$ -matrix approximation, the normal and anomalous self-energies for dilute impurity concentration  $n_{imp} \ll 1$  are given as

$$\hat{\Sigma}^n(i\omega_n) = n_{imp} \hat{T}^b(i\omega_n), \quad (2)$$

$$\hat{\Sigma}^a(i\omega_n) = n_{imp} \hat{T}^b(i\omega_n) \hat{f}(i\omega_n) \hat{T}^b(-i\omega_n), \quad (3)$$

where  $\hat{f}(i\omega_n) \equiv \sum_{\mathbf{k}} \hat{F}_{\mathbf{k}}(i\omega_n) \ll 1$  is the linearized local anomalous Green function.  $\hat{\Sigma}^a$  is diagrammatically expressed in Fig. 1 (a), which expresses the inter-band scattering of a Cooper pair when  $\hat{T}^b$  has off-diagonal elements, as shown in Fig. 1 (b). In the  $s_{\pm}$ -wave state, this inter-band impurity scattering suppresses the superconductivity.

When  $\det\{\hat{I}^b\} \neq 0$ , eq. (1) becomes  $T_{\alpha,\beta}^b = -1/g_{loc,\alpha}^b \cdot \delta_{\alpha,\beta}$  in the unitary limit ( $I \rightarrow \infty$ ), which is band-diagonal even if  $\hat{I}^b$  is not band-diagonal. Therefore, the pair-breaking due to inter-band scattering is absent in the unitary limit unless  $\det\{\hat{I}^b\} = 0$  [3].

On the other hand, Fe-ion substitution in iron pnictides induces the orbital-diagonal local impurity potential. Then,  $\hat{I}^b$  is given as  $\hat{I}_{\mathbf{k},\mathbf{k}'}^b = I \hat{U}_{\mathbf{k}}^\dagger \hat{U}_{\mathbf{k}'}$ , where  $\hat{U}_{\mathbf{k}}$  is the transformation matrix between orbital- and band-bases.

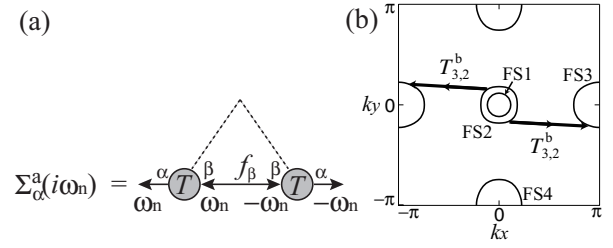


FIG. 1: (a) Diagrammatic expression for  $\hat{\Sigma}^a$ . (b) Inter-band scattering of a Cooper pair described by  $\hat{\Sigma}^a$ .

Because of the large  $\mathbf{k}$ -dependence in iron pnictides,  $\hat{T}^b$  is not diagonal even in the unitary limit, and therefore  $s_{\pm}$ -wave state is fragile against impurities. This is the main result in Ref. [1].

In Comment[2], Bang seems to claim that the bare impurity potential  $\hat{I}^b$  should be subtracted from the  $T$ -matrix  $\hat{T}^b$ . If we follow his comment in eq. (3), inter-band scattering of Cooper pair always occurs. However, such subtraction violates the perturbation theory, and induces various unphysical results, for example, the divergence of  $\hat{\Sigma}^a$  for  $I^b \rightarrow \infty$  will give the divergence of  $T_c$  in the  $s_{++}$  wave state. We agree that the real-part of the "normal self-energy", which becomes  $n_{imp} \hat{I}^b$  in the Born limit [4], is absorbed by the change in the chemical potential. However, this fact never means that  $T$ -matrix is renormalized to  $\hat{T}^b - \hat{I}^b$ , contrary to the claim by Bang.

In the constant  $\hat{I}^b$  model, Bang[2] showed that the  $T$ -matrix is not band-diagonal when  $\hat{I}^b \propto \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ , (*i.e.*

$\det\{\hat{I}^b\} = 0$ ) in the unitary limit. However, this is the special case (measure zero probability) in the statement (iii). In contrast,  $\hat{T}^b$  always has off-diagonal elements in multiorbital models since  $\hat{I}^b$  is not constant. Thus, it is better to analyze the multiorbital model for a quantitative study of impurity effects in iron pnictides.

In summary, our studies of impurity effect in iron pnictides[1] are correctly calculated based on the  $T$ -matrix approximation, which becomes exact in the dilute limit. The replacement  $\hat{T}^b$  with  $\hat{T}^b - \hat{I}^b$  in eq. (3), which was proposed by Bang [2], breaks the perturbation theory and is therefore erroneous.

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- [4] In the presence of the electron-hole symmetry,  $\text{Re}\Sigma^n = \frac{I^b}{1+(\pi N I^b)^2}$  for general  $I^b$ , where  $N$  denotes the density of state on the Fermi energy.